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Journal of Computational and Applied Mathematics 142 (2002) 401–409

JOURNAL OF
COMPUTATIONAL AND
APPLIED MATHEMATICSwww.elsevier.com/locate/cam

On the asymptotic expansion of the entropy of Gegenbauer polynomials

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Received 14 July 2000; received in revised form 14 November 2000

Abstract

In this paper, the third term in the asymptotic expansion of the entropy for orthonormal Gegenbauer polynomials with fixed integer parameter is obtained as the degree of the polynomials tends to infinity, improving the results of Buyarov et al. (J. Phys. A 33 (2000) 6549). © 2002 Elsevier Science B.V. All rights reserved.

Keywords: Gegenbauer polynomials; Shannon entropy; Logarithmic potential

1. Introduction and statement of results

In the last few years much attention has been paid to the study of the Boltzmann–Shannon information entropy

$$S_\rho = - \int \rho(x) \ln(\rho(x)) dx,$$

in connection with quantum mechanical systems (see e.g. [2,6–8,10]). Probably, the most important case is when $\rho(x) = |\Psi(x)|^2$, where $\Psi(x)$ is the wave function of a one-particle system (in the position or momentum space). For many standard models, such as the harmonic oscillator or the hydrogen atom, the wave function can be expressed in terms of some classical orthogonal polynomials (Gegenbauer, Laguerre, Hermite, etc.). This leads to the study of entropy of these families, that is, of functionals of the form

$$S_n(w) = \int_A q_n^2(x) \ln q_n^2(x) dx,$$

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where Δ is an interval on the real axis, w is a weight supported on Δ , and q_n is the corresponding orthonormal polynomial of degree n (see e.g. [5]).

In this paper we deal with the entropy of Gegenbauer polynomials (see [9, Section 4.7]),

$$G_n^\ell(x) = g_{n\ell}x^n + \text{lower degree terms},$$

orthonormal on $\Delta = [-1, 1]$ with respect to the probability density

$$w_\ell(x) = c_\ell(1 - x^2)^{\ell-1/2}, \quad x \in \Delta,$$

where

$$c_\ell = \frac{\Gamma(\ell + 1)}{\sqrt{\pi}\Gamma(\ell + 1/2)}, \quad g_{n\ell} = \frac{2^n\Gamma(n + \ell)}{\Gamma(\ell + 1)} \left(\frac{\ell(n + \ell)\Gamma(2\ell)}{\Gamma(n + 2\ell)n!} \right)^{1/2}.$$

For the sake of brevity, we denote by S_n^ℓ the entropy of the polynomial G_n^ℓ ,

$$S_n^\ell = \int_{\Delta} (G_n^\ell(x))^2 \ln(G_n^\ell(x))^2 w_\ell(x) dx.$$

In [3] a constructive approach to the computation of S_n^ℓ for integer $\ell \geq 2$ has been produced. The procedure is as follows: fixed n , $\ell \in \mathbb{N}$, $\ell \geq 2$, we generate polynomials $P_{-1} = 0$, $P_0 = 1, \dots, P_{2\ell-2}$ using the recurrence relation

$$P_{j+1}(x) = (2\ell - 2j - 3)xP_j(x) - (n + j + 1)(n + 2\ell - j - 1)(1 - x^2)P_{j-1}(x).$$

Let

$$P(x) = P_{2\ell-2}(x) = \alpha_{n\ell} \prod_{j=1}^{2\ell-2} (x - \xi_j)$$

and

$$H(x) = \sum_{j=0}^{2\ell-2} (-1)^j P_{j-1}(x) P_{2\ell-2j-3}(x) = \beta_{n\ell} x^{2\ell-4} + \text{lower degree terms},$$

then the following formula holds:

$$S_n^\ell = s_{n\ell} + r_{n\ell} \sum_{j=1}^{2\ell-2} (1 - \xi_j^2) \left[\frac{H}{P'} \frac{G_{n-1}^{\ell+1}}{G_n^\ell} \right] (\xi_j), \quad (1)$$

where

$$s_{n\ell} = 2 \ln \left(\frac{g_{n\ell}}{2^n} \right) - \frac{n}{n + \ell} + 2n(n + \ell) \frac{\beta_{n\ell}}{\alpha_{n\ell}} + 2n \sum_{j=\ell}^{2\ell-1} \frac{1}{n + j},$$

$$r_{n\ell} = 2(n + \ell) \sqrt{\frac{2(\ell + 1)n(n + 2\ell)}{2\ell + 1}}.$$

The procedure above allowed the authors in [3] to establish that the entropy S_n^ℓ has the following asymptotic expansion as $n \rightarrow \infty$:

$$S_n^\ell = S_\ell + \frac{\gamma_\ell}{n} + O(n^{-2}), \quad S_\ell = 1 + \ln \frac{\Gamma(2\ell)}{\Gamma(\ell)\Gamma(\ell + 1)}. \quad (2)$$

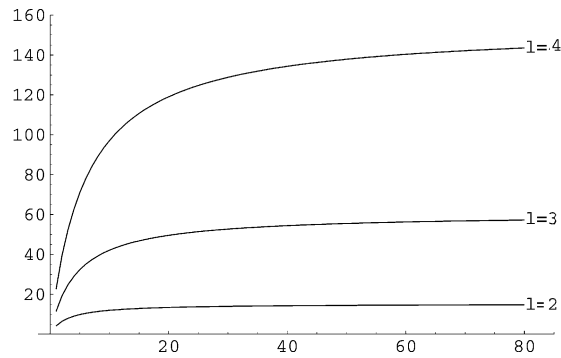


Fig. 1. Plot of $n^2(S_n^\ell - S_\ell - \gamma_\ell/n)$, $n = 1, \dots, 75$, for $\ell = 2, 3, 4$.

Table 1
Values of S_ℓ , γ_ℓ and λ_ℓ for $\ell = 2, 3, 4$

ℓ	S_ℓ	γ_ℓ	λ_ℓ
2	2.09	-5.61	15.18
3	3.30	-14.11	60.50
4	4.56	-26.55	155.13

In fact, the first term S_ℓ was previously found in [1]. The coefficient γ_ℓ can be computed constructing the polynomials $S_{-1} = 0$, $S_0 = 1, \dots, S_{2\ell-2}$ from the recurrence relation

$$S_{j+1}(x) = (2\ell - 2j - 3)S_j(x) - xS_{j-1}(x), \quad S = S_{2\ell-2}, \quad (3)$$

defining

$$R(x) = \sum_{j=0}^{2\ell-2} (-1)^j S_{j-1}(x) S_{2\ell-2j-3}(x)$$

and evaluating

$$\gamma_\ell = -2\ell^2 + \ell - 2 \sum_{j=1}^{\ell-1} A_\ell(\zeta_j), \quad A_\ell(z) = \sqrt{z} \frac{R}{S'}(z) \frac{J_{\ell+1/2}}{J_{\ell-1/2}}(\sqrt{z}), \quad (4)$$

where ζ_j , $j = 1, \dots, \ell - 1$ are the zeros of S (S has degree $\ell - 1$), and J_λ is the Bessel function of order λ .

See Fig. 1, Table 1.

The main goal of this paper is to improve the asymptotic results of [3], finding the next term in the relation (2):

Theorem 1. For $\ell \in \mathbb{N}$, $\ell \geq 2$ the sequence of Gegenbauer entropies has the following asymptotic expansion as $n \rightarrow \infty$:

$$S_n^\ell = S_\ell + \frac{\gamma_\ell}{n} + \frac{\lambda_\ell}{n^2} + O(n^{-3}), \quad (5)$$

where

$$\lambda_\ell = \ell^2(3\ell - 2) + \sum_{j=1}^{\ell-1} [6\ell A_\ell(\zeta_j) - 4\ell \zeta_j A'_\ell(\zeta_j)] \quad (6)$$

and S_ℓ , γ_ℓ and A_ℓ are defined in (2), (4).

2. Proof of Theorem 1

Using the well-known relation

$$G_n^\ell(x) = k_n^\ell T_{n+\ell}^{(\ell)}(x), \quad k_n^\ell = \left[\frac{2}{\pi} \frac{\Gamma(n+1)}{c_\ell(n+\ell)\Gamma(n+2\ell)} \right]^{1/2} > 0,$$

where $T_{n+\ell}^{(\ell)}$ denotes the ℓ th derivative of the Chebyshev polynomial of the first kind of degree $n+\ell$, we can rewrite (1) as

$$S_n^\ell = s_{n\ell} + 2(n+\ell) \sum_{j=1}^{2\ell-2} (1 - \zeta_j^2) \left[\frac{H}{P'} \frac{T_{n+\ell}^{(\ell+1)}}{T_{n+\ell}^{(\ell)}} \right](\zeta_j). \quad (7)$$

In order to obtain (5) and (6), the asymptotic behavior of each term in the formula above, up to $O(n^{-3})$, must be established. We begin by studying the asymptotics of $s_{n\ell}$.

First, it is straightforward to find that

$$2 \ln \left(\frac{g_{n\ell}}{2^n} \right) = \ln \frac{\Gamma(2\ell)}{\Gamma(\ell)\Gamma(\ell+1)} - \frac{\ell(\ell-1)}{n} + \frac{\ell^2(\ell-1)}{n^2} + O(n^{-3}), \quad (8)$$

$$\frac{n}{n+\ell} = 1 - \frac{\ell}{n} + \frac{\ell^2}{n^2} + O(n^{-3}), \quad (9)$$

$$2n \sum_{j=\ell}^{2\ell-1} \frac{1}{n+j} = 2\ell - \frac{\ell(3\ell-1)}{n} + \frac{\ell/3(2\ell-1)(7\ell-1)}{n^2} + O(n^{-3}). \quad (10)$$

In order to compute the asymptotics of $\beta_{n\ell}/\alpha_{n\ell}$, we make use of polynomials p_k , introduced in [3], and connected with P_k by the following relation:

$$P_k(x) = (\sqrt{1-x^2})^k p_k \left(\frac{x}{\sqrt{1-x^2}} \right).$$

Thus, $p_{-1} = 0$, $p_0 = 1$, ..., $p_{2\ell-2}$ can be generated by means of the recurrence relation:

$$p_{k+1}(y) = (2\ell - 2k - 3)y p_k(y) - (n+k+1)(n+2\ell-k-1)p_{k-1}(y). \quad (11)$$

If

$$h_{2\ell-4}(y) = \sum_{j=0}^{2\ell-2} (-1)^j p_{j-1}(y) p_{2\ell-j-3}(y), \quad \deg(h_{2\ell-4}) = 2\ell - 4,$$

then it was established in [3] that

$$\frac{\beta_{n\ell}}{\alpha_{n\ell}} = \frac{h_{2\ell-4}}{p_{2\ell-2}}(i),$$

where $i = \sqrt{-1}$. By (11), the coefficients of $p_k(y)$ depend on n . If

$$p_k(y) = \sum_{j=0}^k a_j^k(n) y^j,$$

then $a_j^k(n) = 0$ for $k - j$ odd, and $a_j^k(n)$ is a polynomial in n of degree $k - j$ for $k - j$ even. Now,

$$\begin{aligned} h_{2\ell-4}(i) &= \sum_{j=0}^{2\ell-2} (-1)^j \sum_{k=0}^{j-1} \sum_{h=0}^{2\ell-j-3} a_k^{j-1}(n) a_h^{2\ell-j-3}(n) i^{k+h} \\ &= \sum_{j=0}^{\ell-2} (a_0^{2j}(n) a_0^{2\ell-2j-4}(n) - 2a_2^{2j}(n) a_0^{2\ell-2j-4}(n) + a_1^{2j+1}(n) a_1^{2\ell-2j-5}(n)) + O(n^{2\ell-8}). \end{aligned} \quad (12)$$

From (11) it follows (see [3, Proposition 2]) that the polynomials p_j satisfy the relation

$$(n + j + 1)(n + 2\ell - j - 1) p_{j-1} p_{2\ell-j-3} + p_j p_{2\ell-j-2} = (-1)^j p_{2\ell-2},$$

for $j = 0, \dots, 2\ell - 2$. Replacing j by $2j + 1$ in the above equation, it is easy to obtain that:

$$-a_0^{2\ell-2}(n) = (n + 2j + 2)(n + 2\ell - 2j - 2) a_0^{2j}(n) a_0^{2\ell-2j-4}(n). \quad (13)$$

In particular,

$$\sum_{j=0}^{\ell-2} a_0^{2j}(n) a_0^{2\ell-2j-4}(n) = -a_0^{2\ell-2}(n) \sum_{j=0}^{\ell-2} \frac{1}{(n + 2j + 2)(n + 2\ell - 2j - 2)}. \quad (14)$$

Let c_j^k denotes the leading coefficient of the polynomial $a_j^k(n)$:

$$a_j^k(n) = c_j^k n^{k-j} + \text{lower degree terms}.$$

Then, by (14),

$$\begin{aligned} &\frac{1}{p_{2\ell-2}(i)} \sum_{j=0}^{\ell-2} a_0^{2j}(n) a_0^{2\ell-2j-4}(n) \\ &= - \left(1 + \frac{c_2^{2\ell-2}}{c_0^{2\ell-2}} \frac{1}{n^2} + O(n^{-3}) \right) \sum_{j=0}^{\ell-2} \frac{1}{(n + 2j + 2)(n + 2\ell - 2j - 2)}. \end{aligned} \quad (15)$$

In the same fashion,

$$\begin{aligned} &\frac{1}{p_{2\ell-2}(i)} \sum_{j=0}^{\ell-2} (-2a_2^{2j}(n) a_0^{2\ell-2j-4}(n) + a_1^{2j+1}(n) a_1^{2\ell-2j-5}(n)) \\ &= \frac{1}{c_0^{2\ell-2} n^4} \sum_{j=0}^{\ell-2} (-2c_2^{2j} c_0^{2\ell-2j-4} + c_1^{2j+1} c_1^{2\ell-2j-5}) + O(n^{-5}). \end{aligned} \quad (16)$$

In order to compute explicit values of c_0^{2k} , c_1^{2k+1} and c_2^{2k+2} we use the following relation which is a straightforward consequence of (11):

$$a_j^{k+1}(n) = (2\ell - 2k - 3)a_{j-1}^k(n) - (n + k + 1)(n + 2\ell - k - 1)a_j^{k-1}(n), \quad (17)$$

for $j = 0, \dots, k + 1$ ($a_j^k(n) = 0$ for $j > k$, $a_{-1}^k(n) = 0$).

Proposition 2.

$$c_0^{2k} = (-1)^k, \quad (18)$$

$$c_1^{2k+1} = (-1)^k(k + 1)(2\ell - 2k - 3), \quad (19)$$

$$c_2^{2k} = (-1)^{k-1}2k(k + 1)(k - \ell + 1/2)(k - \ell + 3/2). \quad (20)$$

Proof. Comparing the leading coefficient in (17) with $j = 0$ it is obtained that $c_0^{2k+2} = -c_0^{2k}$. Since $c_0^0 = 1$, we get (18). On the other hand, the same procedure and (18) yields

$$c_1^{2k+1} = (-1)^k(2\ell - 4k - 3) - c_1^{2k-1}. \quad (21)$$

Now since $c_1^1 = 2\ell - 3$, (19) can be proved easily by induction on k using (21).

Finally, taking the leading coefficient in (17) with $j = 2$ and using (19) one obtains that

$$c_2^{2k+2} = (-1)^k(8k^3 + (-12\ell + 30)k^2 + (4\ell^2 - 28\ell + 37)k + (4\ell^2 - 16\ell + 15)) - c_2^{2k}. \quad (22)$$

Since $c_2^2 = 4\ell^2 - 16\ell + 15 = (2\ell - 5)(2\ell - 3)$, (20) can be proved by induction on k using (22). This completes the proof. \square

Relations (12), (15), (16) and (18)–(20) give

$$\begin{aligned} 2n(n + \ell) \frac{\beta_{n\ell}}{\alpha_{n\ell}} &= \left(1 + \frac{c_2^{2\ell-2}}{c_0^{2\ell-2}} \frac{1}{n^2} + O(n^{-3})\right) \sum_{j=0}^{\ell-2} \frac{-2n(n + \ell)}{(n + 2j + 2)(n + 2\ell - 2j - 2)} \\ &\quad + \frac{2n(n + \ell)}{c_0^{2\ell-2}n^4} \sum_{j=0}^{\ell-2} (-2c_2^{2j}c_0^{2\ell-2j-4} + c_1^{2j+1}c_1^{2\ell-2j-5}) + O(n^{-5}) \\ &= -2\ell + 2 + \frac{2\ell(\ell - 1)}{n} - \frac{1}{3}\ell(\ell - 1)(8\ell - 1)\frac{1}{n^2} + O(n^{-3}). \end{aligned} \quad (23)$$

Gathering (8)–(10) and (23) we obtain that the coefficient of n^{-2} in the expansion of $s_{n\ell}$ is $\ell^2(3\ell - 2)$.

Now we study the term $2(n + \ell) \sum_{j=1}^{2\ell-2} (1 - \xi_j^2)[(H/P')(T_{n+\ell}^{(\ell+1)}/T_{n+\ell}^{(\ell)})](\xi_j)$. The formula of Mehler-Heine [9, Section 8.1] gives

$$\lim_{n \rightarrow \infty} T_{n+\ell} \left(1 - \frac{z}{2n^2}\right) = \cos(\sqrt{z}) = \sqrt{\pi/2} z^{1/4} J_{-1/2}(\sqrt{z}).$$

In fact, using the explicit expression for T_n , it is not difficult to get that the limit

$$\lim_{n \rightarrow \infty} n \left[T_{n+\ell} \left(1 - \frac{z}{2n^2}\right) - \sqrt{\pi/2} z^{1/4} J_{-1/2}(\sqrt{z}) \right] = -\ell \sqrt{z} \sin(\sqrt{z}) = -\ell \sqrt{\pi/2} z^{3/4} J_{1/2}(\sqrt{z}), \quad (24)$$

holds locally uniformly in \mathbb{C} . Moreover

$$n \left[T_{n+\ell} \left(1 - \frac{z}{2n^2}\right) - \sqrt{\pi/2} z^{1/4} J_{-1/2}(\sqrt{z}) \right]$$

is a sequence of analytic functions, and by Weierstrass' theorem (see [4, Chapter VII, Theorem 2.1]), we can take derivatives in (24) with respect to z , k times:

$$\begin{aligned} \lim_{n \rightarrow \infty} n \left[n^{-2k} T_{n+\ell}^{(k)} \left(1 - \frac{z}{2n^2} \right) - \sqrt{\frac{\pi}{2}} z^{-k/2+1/4} J_{k-1/2}(\sqrt{z}) \right] \\ = \ell \sqrt{\frac{\pi}{2}} z^{-k/2+1/4} (2k J_{k-1/2}(\sqrt{z}) - \sqrt{z} J_{k+1/2}(\sqrt{z})), \end{aligned}$$

so that finally

$$\begin{aligned} n^{-2} \frac{T_{n+\ell}^{(\ell+1)}}{T_{n+\ell}^{(\ell)}} \left(1 - \frac{z}{2n^2} \right) &= \frac{1}{\sqrt{z}} \frac{J_{\ell+1/2}}{J_{\ell-1/2}}(\sqrt{z}) \\ &+ \frac{1}{n} \left(\frac{\ell}{\sqrt{z}} \frac{J_{\ell+1/2}}{J_{\ell-1/2}}(\sqrt{z}) + 2\ell \sqrt{z} \left(\frac{J_{\ell+1/2}}{J_{\ell-1/2}}(\sqrt{z}) \right)' \right) + O(n^{-2}). \end{aligned} \quad (25)$$

By proposition 4 of [3],

$$\begin{aligned} \lim_{n \rightarrow \infty} P_j \left(1 - \frac{z}{2n^2} \right) &= S_j(z), \\ \lim_{n \rightarrow \infty} \frac{1}{2n^2} P_j' \left(1 - \frac{z}{2n^2} \right) &= -S_j'(z), \end{aligned} \quad (26)$$

locally uniformly in \mathbb{C} for $j = 0, \dots, 2\ell - 2$. We need more:

Proposition 3. For $j = 0, \dots, 2\ell - 2$,

$$\lim_{n \rightarrow \infty} n \left[P_j \left(1 - \frac{z}{2n^2} \right) - S_j(z) \right] = 2\ell z S_j'(z), \quad (27)$$

$$\lim_{n \rightarrow \infty} n \left[\frac{1}{2n^2} P_j' \left(1 - \frac{z}{2n^2} \right) + S_j'(z) \right] = -2\ell S_j'(z) - 2\ell z S_j''(z), \quad (28)$$

locally uniformly in \mathbb{C} .

Proof. We prove that (27) holds locally uniformly in \mathbb{C} , by induction on j ; then (28) is obtained taking derivatives in (27). For $j = 0$ and $j = 1$, (27) holds trivially since $S_0(z) = 1$ and $S_1(z) = 2\ell - 3$. Also

$$\begin{aligned} n \left(P_{j+1} \left(1 - \frac{z}{2n^2} \right) - S_{j+1}(z) \right) &= (2\ell - 2j - 3)n \left(P_j \left(1 - \frac{z}{2n^2} \right) - S_j(z) \right) \\ &\quad - zn \left(P_{j-1} \left(1 - \frac{z}{2n^2} \right) - S_{j-1}(z) \right) \\ &\quad - 2\ell z P_{j-1} \left(1 - \frac{z}{2n^2} \right) + O(n^{-2}). \end{aligned}$$

Taking the limit as $n \rightarrow \infty$, using the induction hypothesis and (26) we obtain:

$$\lim_{n \rightarrow \infty} n \left(P_{j+1} \left(1 - \frac{z}{2n^2} \right) - S_{j+1}(z) \right) = 2\ell z [(2\ell - 2j - 3)S'_j(z) - zS'_{j-1}(z) - S_{j-1}(z)],$$

locally uniformly in \mathbb{C} . The proof is concluded by taking derivatives in (3). \square

It is also easy to prove that

$$H \left(1 - \frac{z}{2n^2} \right) = R(z) + 2\ell z R'(z) \frac{1}{n} + O(n^{-2}),$$

and as a consequence,

$$n^2 \frac{H}{P'} \left(1 - \frac{z}{2n^2} \right) = -\frac{R}{2S'}(z) + \frac{\ell}{n} \left(\frac{R}{S'}(z) - z \left(\frac{R}{S'} \right)' \right) + O(n^{-2}). \quad (29)$$

Observe that P depends on n , ℓ and that P is symmetric with respect to the origin. Its zeros $\xi_{j,n}$ can be written as

$$\xi_{j,n} = (-1)^j - \frac{\zeta_j(n)}{2n^2}, \quad \zeta_{2j-1}(n) = -\zeta_{2j}(n)$$

and satisfy

$$\lim_{n \rightarrow \infty} \zeta_{2j}(n) = \zeta_j, \quad j = 1, \dots, \ell - 1,$$

$$\lim_{n \rightarrow \infty} n^2(1 - \xi_{2j,n}^2) = \zeta_j, \quad j = 1, \dots, \ell - 1.$$

Also, using (27) and taking into account that $S(\zeta_j) = 0$, for $j = 1, \dots, \ell - 1$ we get

$$\begin{aligned} \lim_{n \rightarrow \infty} n[n^2(1 - \xi_{2j,n}^2) - \zeta_j] &= \lim_{n \rightarrow \infty} n(\zeta_{2j}(n) - \zeta_j) \\ &= \lim_{n \rightarrow \infty} \frac{\zeta_{2j}(n) - \zeta_j}{S(\zeta_{2j}(n)) - S(\zeta_j)} n(S(\zeta_{2j}(n)) - S(\zeta_j)) \\ &= \frac{1}{S'(\zeta_j)} \lim_{n \rightarrow \infty} nS(\zeta_{2j}(n)) \\ &= \frac{-1}{S'(\zeta_j)} \lim_{n \rightarrow \infty} n \left[P \left(1 - \frac{\zeta_{2j}(n)}{2n^2} \right) - S(\zeta_{2j}(n)) \right] = -2\ell \zeta_j. \end{aligned} \quad (30)$$

Finally, from (30), (29) and (25) we can obtain the coefficient of n^{-2} in the second term in (7):

$$\ell \sum_{j=1}^{\ell-1} [6A(\zeta_j) - 4\zeta_j A'(\zeta_j)],$$

which concludes the proof. \square

Acknowledgements

The author wishes to thank Prof. A. Martínez Finkelshtein for the statement of the problem and for his suggestions, comments and help. He is also indebted to the anonymous referee for a careful reading of the manuscript.

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